

# Understanding Ozone Pollution:

## A Comparison of Chemical Mechanisms

Jane Coates and Tim Butler

### Motivation

- ▶ Importance of  $O_3$  production chemistry representation – future emission scenarios.
- ▶ Compare different  $O_3$  chemistry representations used in chemical transport models.
- ▶ Determine effects on  $O_3$  production by comparing treatment of Volatile Organic Compounds (VOCs) degradation products.

### Approach

- ▶ Tagged Ozone Production Potentials (TOPPs) [1] calculated over 7 days for VOCs common to urban environments.

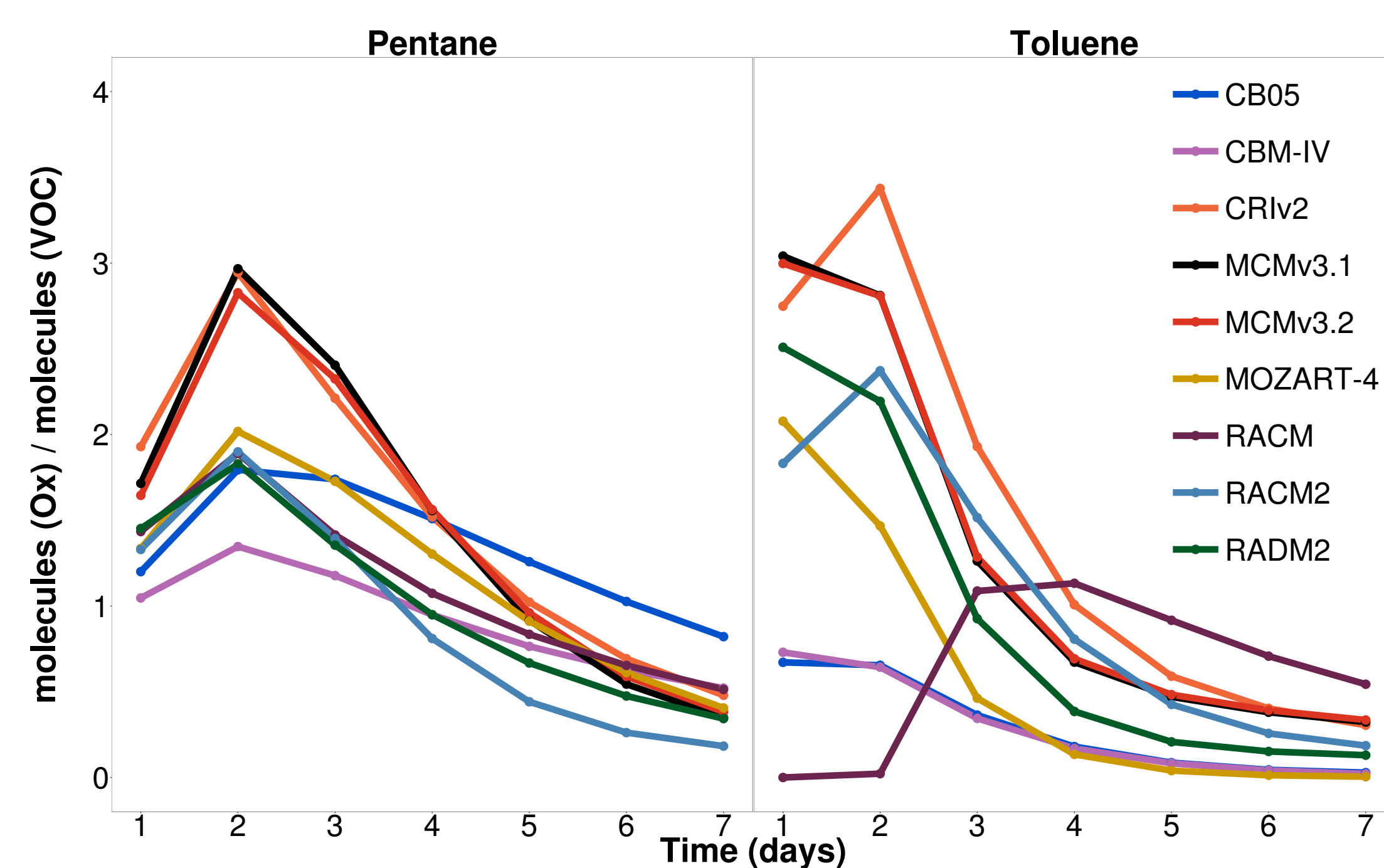
- ▶ Following mechanisms are compared to near-explicit MCM v3.2.

|          |        |        |          |
|----------|--------|--------|----------|
| MCM v3.1 | CRI v2 | CBM-IV | CB05     |
| RADM2    | RACM   | RACM2  | MOZART-4 |

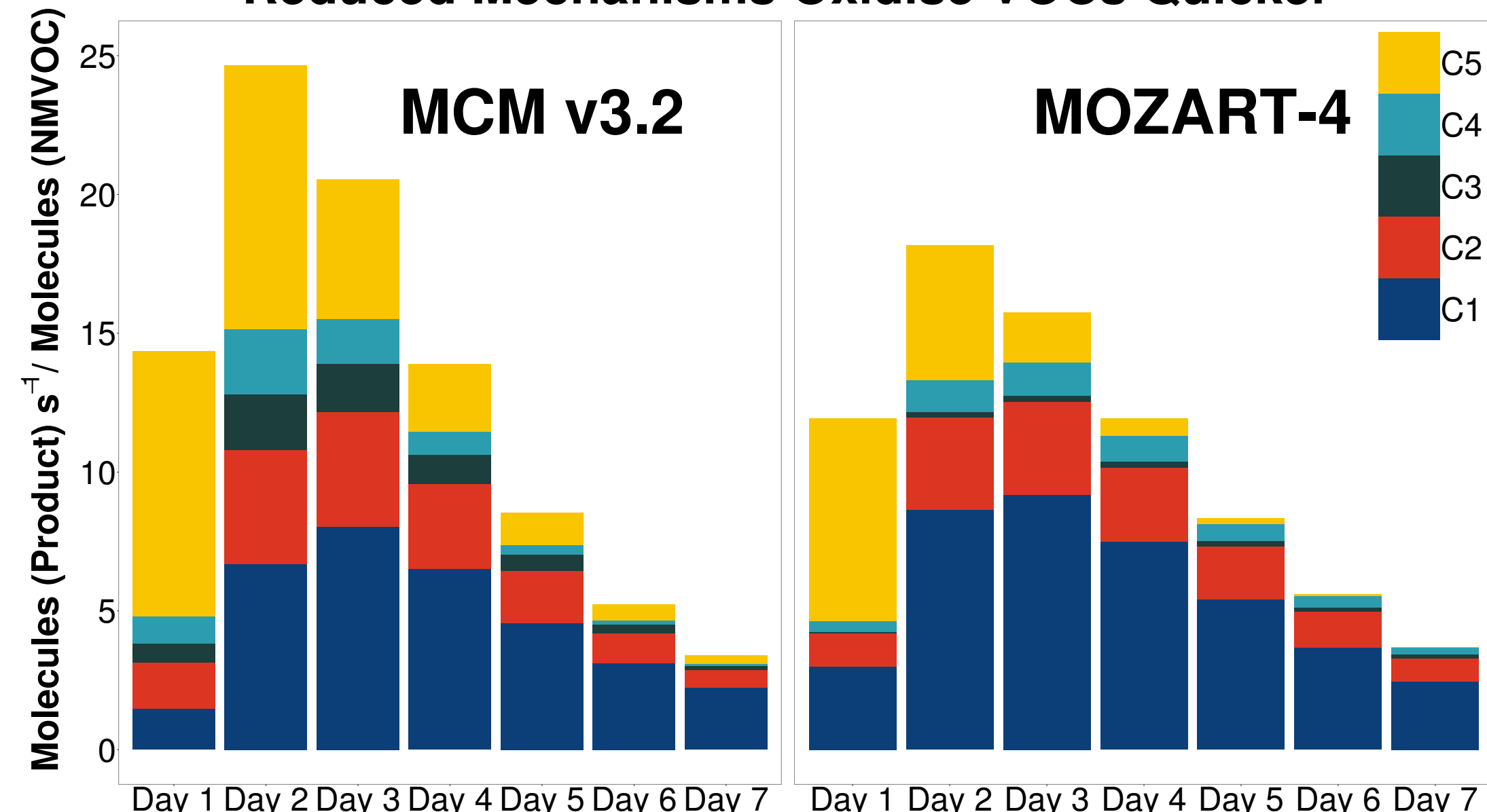
- ▶  $O_x$  ( $= O_3 + NO_2$ ) production allocated to emitted VOC by 'tagging' its organic degradation products.

### Results

#### TOPP Time Series: Large Spread between Mechanisms

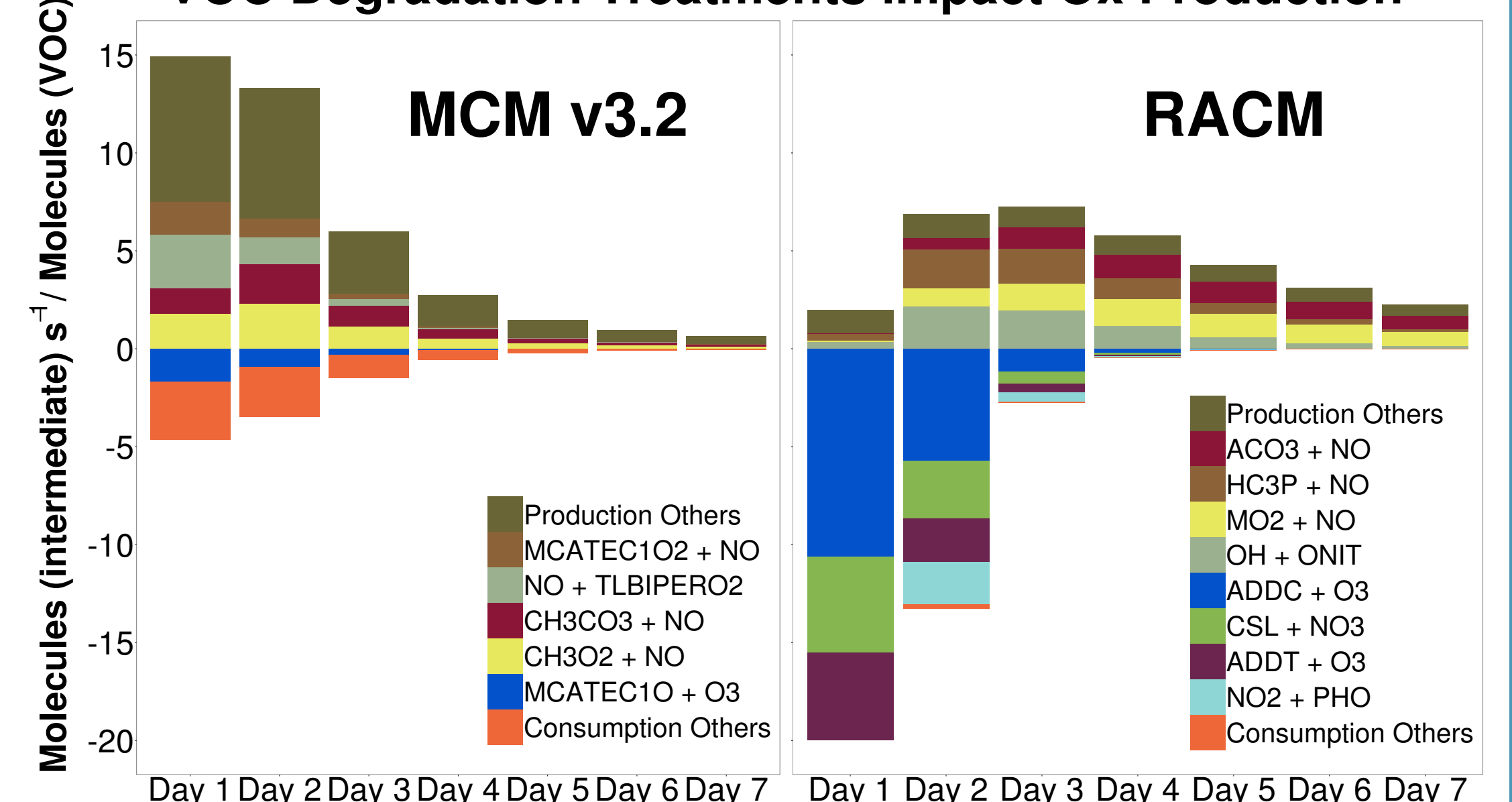


#### Pentane Ox Production by Carbon Number: Reduced Mechanisms Oxidise VOCs Quicker



#### Toluene Organic Ox Budgets:

#### VOC Degradation Treatments impact Ox Production



### Conclusions

- ▶ Near-explicit mechanisms produce more  $O_x$  than less-explicit mechanisms.
- ▶ VOCs broken down into smaller fragments quicker in less-explicit mechanisms resulting in less  $O_x$  production.
- ▶ First day  $O_x$  production from VOCs similar between many mechanisms, larger differences over time.
- ▶ Differences in VOC degradation treatments impacts  $O_x$  production – RACM aromatic chemistry.

### References

- [1] T. M. Butler, M. G. Lawrence, D. Taraborrelli, and J. Lelieveld. Multi-day ozone production potential of volatile organic compounds calculated with a tagging approach. Atmospheric Environment, 45(24):4082–4090, 2011.



### The IASS is sponsored by

